# Molecular dynamics simulation of DNA-directed assembly of nanoparticle superlattices using patterned templates

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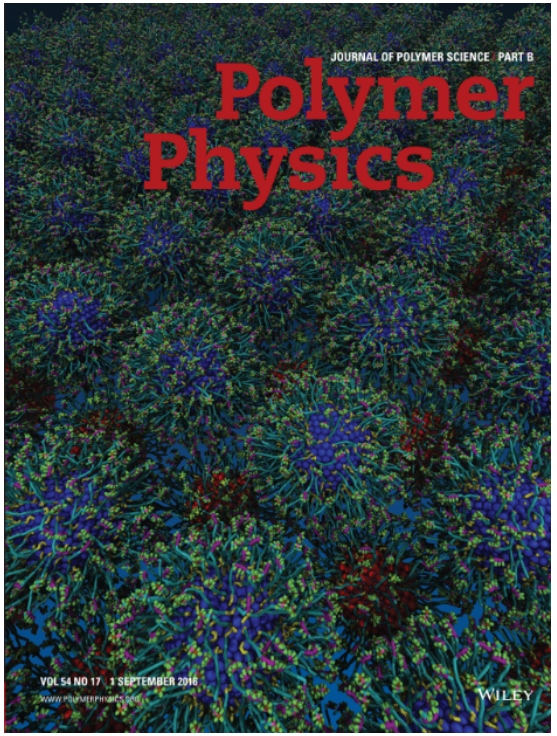
Epitaxial growth of DNA functionalized nanoparticles is used to grow extended superlattices with a controllable orientation for optimizing the physical properties of the materials. However, structural defects exist in epitaxial layers. To understand the origin of the defects, we use a coarse-grained molecular dynamics simulation to investigate the growth of DNA-coated nanoparticles on a nano-patterned substrate. Design rules are developed to minimize the defect formation, which will open the door to constructing large-scale, defect-free superlattices for real applications.




**Cover image**: simulation results of a well-ordered epitaxial layer for an optimized template.

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